10th Anniversary of Catalysts: Achievements in Computational Catalysis Techniques and Applications

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Deadline for manuscript submissions:
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Message from the Guest Editors

In 2021, Catalysts will reach a significant milestone in its history by welcoming its tenth anniversary. In order to celebrate this special occasion, we will be launching a Special Issue entitled "10th Anniversary of Catalysts: Achievements in Computational Catalysis Techniques and Applications."

Computational catalysis has emerged as one of the fastest growing research fields in the last decade, and it now represents a critical tool for the analysis of chemical mechanisms and active sites. As the field of computational catalysis continues to expand, the gap between models and reality is beginning to narrow. We are particularly interested in articles that investigate the secondary effects influencing catalysis and reaction mechanisms. This includes the role of structural defects, the solvation environment or neighbor-neighbor effects, deactivation events, and work that incorporates system features encountered at finite temperatures. Furthermore, we are interested in new techniques and applications that enable extended time scale analyses, as well as high throughput screening techniques that involve machine learning or descriptor-based protocols.

Special Issue